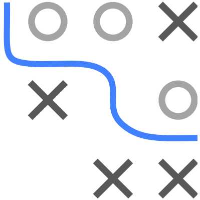
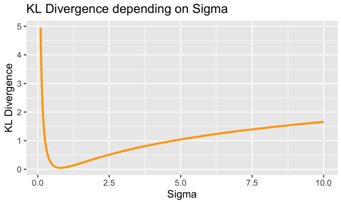
Introduction to Machine Learning

Kullback-Leibler Divergence





Learning goals

- Know the KL divergence as distance between distributions
- Understand KL as expected log-difference
- Understand how KL can be used as loss
- Understand that KL is equivalent to the expected likelihood ratio

KULLBACK-LEIBLER DIVERGENCE

We now want to establish a measure of distance between (discrete or continuous) distributions with the same support for $X \sim p(X)$:

$$D_{KL}(p\|q) = \mathbb{E}_{X\sim p}\left[\log \frac{p(X)}{q(X)}\right] = \sum_{x\in\mathcal{X}} p(x)\cdot \log \frac{p(x)}{q(x)},$$

or:

$$D_{KL}(p\|q) = \mathbb{E}_{X\sim p}\left[\log \frac{p(X)}{q(X)}\right] = \int_{x\in\mathcal{X}} p(x)\cdot \log \frac{p(x)}{q(x)}\mathrm{d}x.$$

In the above definition, we use the conventions that $0\log(0/0) = 0$, $0\log(0/q) = 0$ and $p\log(p/0) = \infty$ (based on continuity arguments where $p \to 0$). Thus, if there is any realization $x \in \mathcal{X}$ such that $p(x) > 0$ and $q(x) = 0$, then $D_{KL}(p\|q) = \infty$.

KULLBACK-LEIBLER DIVERGENCE / 2

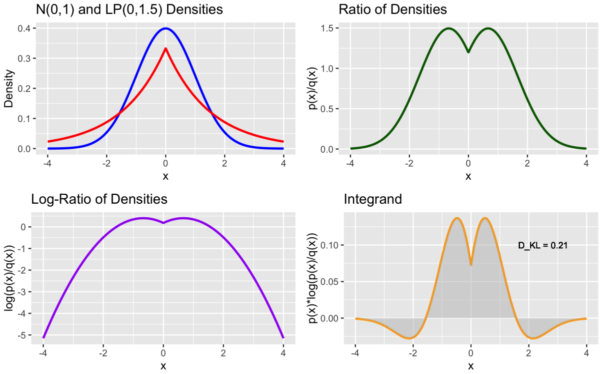
$$D_{KL}(p\|q) = \mathbb{E}_{X\sim p}\left[\log \frac{p(X)}{q(X)}\right]$$

- What is the intuition behind this formula?
- We will soon see that KL has quite some value in measuring "differences" but is not a true distance.
- We already see that the formula is not symmetric and it often makes sense to think of p as the first or original form of the data, and q as something that we want to measure the quality of with reference to p.

KL-DIVERGENCE EXAMPLE

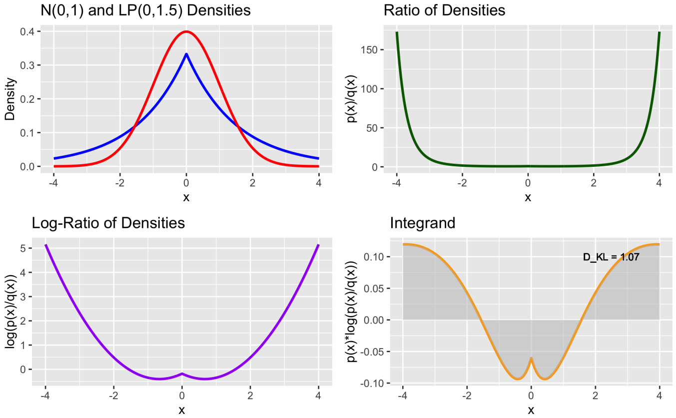
KL divergence between $p(x) = N(0, 1)$ and $q(x) = LP(0, 1.5)$ given by

$$D_{KL}(p\|q) = \int_{x \in \mathcal{X}} p(x) \cdot \log \frac{p(x)}{q(x)}.$$



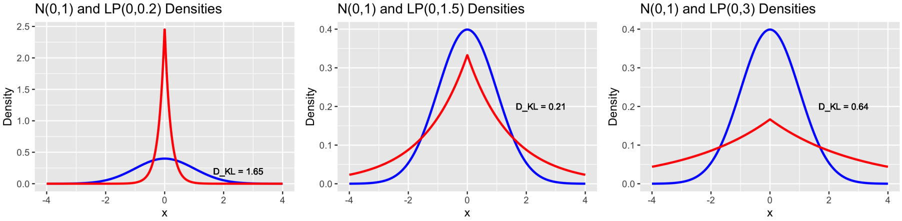
KL-DIVERGENCE EXAMPLE

KL divergence between $p(x) = LP(0, 1.5)$ and $q(x) = N(0, 1)$ is different since KL not symmetric



KL-DIVERGENCE EXAMPLE

KL divergence of $p(x) = N(0,1)$ and $q(x) = LP(0,\sigma)$ for varying σ



INFORMATION INEQUALITY

$D_{KL}(p\|q) \geq 0$ holds always true for any pair of distributions, and holds with equality if and only if $p = q$.

We use Jensen's inequality. Let A be the support of p:

$$
\begin{aligned}
-D_{KL}(p\|q) &= -\sum_{x \in A} p(x) \log \frac{p(x)}{q(x)} \\
&= \sum_{x \in A} p(x) \log \frac{q(x)}{p(x)} \\
&\leq \log \sum_{x \in A} p(x) \frac{q(x)}{p(x)} \\
&\leq \log \sum_{x \in \mathcal{X}} q(x) = log(1) = 0
\end{aligned}
$$

As $\log$ is strictly concave, Jensen also tells us that equality can only happen if $q(x)/p(x)$ is constant everywhere. That implies $p = q$.

KL AS LOG-DIFFERENCE

Suppose that data is being generated from an unknown distribution $p(x)$ and we model $p(x)$ using an approximating distribution $q(x)$.

First, we could simply see KL as the expected log-difference between $p(x)$ and $q(x)$:

$$D_{KL}(p\|q) = \mathbb{E}_{X\sim p}[\log(p(X)) - \log(q(X))].$$

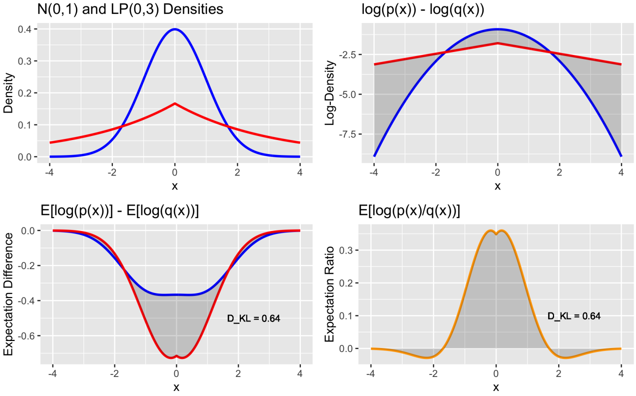
This is why we integrate out with respect to the data distribution p. A "good" approximation $q(x)$ should minimize the difference to $p(x)$.

$$\boxed{x \sim p(x)} \xrightarrow{x} \boxed{\log p(x) - \log q(x)}$$

KL AS LOG-DIFFERENCE / 2

Let $p(x) = N(0,1)$ and $q(x) = LP(0,3)$. Observe

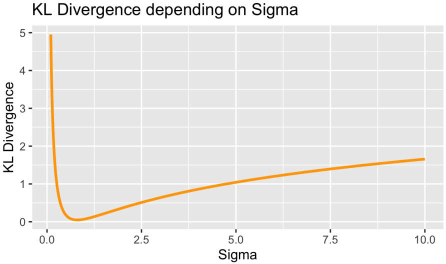
$$
\begin{aligned}
D_{KL}(p \| q) &= \mathbb{E}_{X \sim p}[\log(p(X)) - \log(q(X))] \\
&= \mathbb{E}_{X \sim p}[\log(p(X))] - \mathbb{E}_{X \sim p}[\log(q(X))].
\end{aligned}
$$



KL IN FITTING

In machine learning, KL divergence is commonly used to quantify how different one distribution is from another.
Because KL quantifies the difference between distributions, it can be used as a loss function between distributions.

In our example, we investigated the KL between $p = N(0, 1)$ and $q = LP(0, \sigma)$. Now, we identify an optimal σ which minimizes the KL.



KL AS LIKELIHOOD RATIO

- Let us assume we have some data and want to figure out whether $p(x)$ or $q(x)$ matches it better.
- How do we usually do that in stats? Likelihood ratio!

$$LR = \prod_i \frac{p(\mathbf{x}^{(i)})}{q(\mathbf{x}^{(i)})} \qquad LLR = \sum_i \log \frac{p(\mathbf{x}^{(i)})}{q(\mathbf{x}^{(i)})}$$

If for $\mathbf{x}^{(i)}$ we have $p(\mathbf{x}^{(i)})/q(\mathbf{x}^{(i)}) > 1$, then p seems better, for $p(\mathbf{x}^{(i)})/q(\mathbf{x}^{(i)}) < 1$ q seems better.

- Now assume that the data is generated by p. Can also ask:
- "How to quantify how much better does p fit than q, on average?"

$$\mathbb{E}_p \left[\log \frac{p(X)}{q(X)} \right]$$

That expected LLR is really KL!